

Quantum Particle Dynamics in a Highly Singular 1D-Potential $U(x) = -\alpha\delta(x) + \beta\delta'(x)$ Superposed on a Well-Behaved One

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Abstract

We examine the one-dimensional quantum dynamics of a Schrödinger particle in a potential represented by a generalized function of the form $U(x) = -\alpha\delta(x) + \beta d(\delta(x))/dx$ superposed on a well behaved potential $V(x)$. In this, we construct the full, exact Green's function for such a 1D system analytically in closed form, taking account of a spatially variable mass $m(x)$. Our result shows that there can be no electron transmissions through the $\beta\delta'(x)$ - potential, regardless of the presence of the $V(x)$ - potential and $\alpha\delta(x)$, (with $\alpha \neq 0$).

1 Introduction¹⁻⁵

The advent and rapid development of the fabrication of low dimensional semiconductor materials, replete with the promise of nanostructures upon which a whole new generation of quantum electronic and optical devices can be based, has stimulated an enormous effort to explore the physical properties of such materials, and how they can be manipulated to greatest advantage. Practically all the fields of science and engineering are involved in this massive effort throughout the world. Mathematical modelling has an important role in this matter, enabling analyses that provide insight into the quantum mechanical behavior of nanostructures and their possible optimization. One avenue of such studies over the past quarter century has been the introduction of generalized functions into the potential involved in nonrelativistic one-dimensional Schrödinger dynamics, in particular, the Dirac delta function and its derivative. The inclusion of the Dirac delta function ($\delta(x)$) itself as a potential has proven to be quite straightforward; however, the inclusion of its derivative ($\delta'(x)$) has brought forth substantial controversy. As far back as 1986, Seba⁴ found that electron transmission through that highly singular potential could not take place. However, other researchers have appended boundary conditions to $\delta'(x)$ and claimed that electron transmission can occur.

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We recently studied this problem by constructing the full, exact Green's function for the Dirac-delta-function-derivative model, defining it solely in terms of the usual derivative property [$\delta'(x) \equiv d(\delta(x))/dx$] under integration by parts, with no appeal to additional boundary conditions. Aside from such an integration by parts, we employ only the conventional, well established properties of the Dirac delta function, $\delta(x)$, in terms of integration (as a generalized function), $\int_{-\infty}^{\infty} dx \delta(x-a)f(x) = f(a)$, and differentiation, $d(\eta_+(x-a))/dx = \delta(x-a)$, where $\eta_+(x)$ is the Heaviside unit step function (which is understood to have the value $\eta_+(0) = 1/2$, to which a Fourier series representation converges at the position of the step). Our avoidance of boundary conditions is due to the fact that they are not at all necessary under the usual conventions and that they may distort the meaning of $\delta'(x)$ beyond recognition. The Green's function we obtain analytically in closed form confirms Seba's finding that there can be no electron transmission through the $\delta'(x)$ -singular potential if the potential profile is otherwise well-behaved, and that such a wave-packet must be totally reflected.

In the present paper we extend these one-dimensional considerations to take into account a spatially variable mass, $m(x)$, and a reasonably well behaved spatially variable potential, $V(x)$, and a $\delta(x)$ -potential, all in addition to the $\delta'(x)$ -potential previously examined. It is in this very general situation that we construct the full, exact Schrödinger Green's function in closed form, and show that *no* electron wave packet transmission through $\delta'(x)$ can occur. Our analysis of this problem is in agreement with aspects of the formulation by Park¹⁴, but the later is quite limited in application to one specific case.

2 Derivation of the Exact One-Dimensional Green's Function

Allowing for a variable mass, $m(x)$, the one-dimensional Schrödinger Green's function equation for a system with time-translational invariance has the Sturm-Liouville form in frequency representation $t - t' \rightarrow \omega$ and we suppress the explicit appearance of ω , so $G(x, x'; t - t') \rightarrow G(x, x'; \omega) \equiv G(x, x')$ as given by¹⁶

$$\left[\frac{\partial}{\partial x} \left(\frac{1}{m(x)} \frac{\partial}{\partial x} \right) + V(x) + U(x) \right] G(x, x') = \delta(x - x'). \quad (1)$$

Here, $V(x)$ is understood to be a relatively well behaved potential (which can accommodate finite discontinuities using the well known Green's function joining technique employed in the theory of surface/interface states¹⁷⁻²¹; it also includes an ω - term from the Fourier time-transform) and all highly singular delta-function-type potentials are relegated to $U(x)$ as

$$U(x) = -\alpha\delta(x) + \beta\delta'(x) \quad (2)$$

(α, β are constants and $\delta'(x) \equiv d(\delta(x))/dx$).

To start, we define an auxiliary Green's function, $G_0(x, x')$, as the inverse of the Sturm-Liouville operator excluding $U(x)$:

$$\left[\frac{\partial}{\partial x} \left(\frac{1}{m(x)} \frac{\partial}{\partial x} \right) + V(x) \right] G_0(x, x') = \delta(x - x') \quad (3)$$

Taking $y_1(x)$ and $y_2(x)$ as two linearly independent solutions of the homogeneous counterpart of Eq. (3), with y_1 chosen to satisfy the boundary condition at the lower limit and y_2 doing so at

the upper limit, the solution of Eq.(3) is known to be

$$G_0(x, x') = \frac{m(x')}{\Delta(y_1, y_2)} \begin{cases} y_1(x)y_2(x') & \text{for } x < x' \\ y_2(x)y_1(x') & \text{for } x > x' \end{cases}, \quad (4)$$

where $\Delta(y_1, y_2)$ is the Wronskian of the two solutions, $y_1(x'), y_2(x')$, evaluated at x' :

$$\Delta(y_1, y_2) = \det \begin{vmatrix} y_1 & y_1' \\ y_2 & y_2' \end{vmatrix}, \quad (5)$$

($y' \equiv dy(x')/dx'$).

Considering y_1, y_2 to be known and hence G_0 is known, Eq. (1) may be rewritten as

$$G(x, x') = G_0(x, x') + \int dx'' G_0(x, x'') U(x'') G(x'', x'), \quad (6)$$

or

$$G(x, x') = G_0(x, x') - \alpha G_0(x, 0) G(0, x') + \beta \int dx'' \delta'(x'') G_0(x, x'') G(x'', x'). \quad (7)$$

Integrating by parts, this becomes

$$G(x, x') = G_0(x, x') - \alpha G_0(x, 0) G(0, x') - \beta \int dx'' \delta(x'') \frac{\partial}{\partial x''} [G_0(x, x'') G(x'', x')]. \quad (8)$$

Introducing the notation

$$\begin{aligned} \frac{\partial}{\partial x''} G(x'', x') &\equiv [\partial_{(L)} G(x'', x')]; \quad \frac{\partial}{\partial x''} G(x', x'') \equiv [\partial_{(R)} G(x', x'')]; \\ \frac{\partial}{\partial x'} \frac{\partial}{\partial x''} G(x', x'') &\equiv [\partial_{(L,R)}^2 G(x', x'')]. \end{aligned} \quad (9)$$

Eq.(8) may be written as

$$\begin{aligned} G(x, x') &= G_0(x, x') - \alpha G_0(x, 0) G(0, x') - \beta [\partial_{(R)} G_0(x, 0)] G(0, x') \\ &\quad - \beta G_0(x, 0) [\partial_{(L)} G(0, x')]. \end{aligned} \quad (10)$$

To solve, we need to determine $G(0, x')$ and $[\partial_{(L)} G(0, x')]$: Setting $x \rightarrow 0$, we obtain Eq.(10) as

$$\begin{aligned} G(0, x') &= G_0(0, x') - \alpha G_0(0, 0) G(0, x') - \beta [\partial_{(R)} G_0(0, 0)] G(0, x') \\ &\quad - \beta G_0(0, 0) [\partial_{(L)} G(0, x')]. \end{aligned} \quad (11)$$

Forming the left derivative of Eq.(10), we have

$$\begin{aligned} [\partial_{(L)} G(x, x')] &= [\partial_{(L)} G_0(x, x')] - \alpha [\partial_{(L)} G_0(x, 0)] G(0, x') \\ &\quad - \beta [\partial_{(L,R)}^2 G_0(x, 0)] G(0, x') - \beta [\partial_{(L)} G_0(x, 0)] [\partial_{(L)} G(0, x')], \end{aligned} \quad (12)$$

and putting $x \rightarrow 0$ in Eq.(12), we have

$$\begin{aligned} [\partial_{(L)} G(0, x')] &= [\partial_{(L)} G_0(0, x')] - \alpha [\partial_{(L)} G_0(0, 0)] G(0, x') \\ &\quad - \beta [\partial_{(L,R)}^2 G_0(0, 0)] G(0, x') - \beta [\partial_{(L)} G_0(0, 0)] [\partial_{(L)} G(0, x')]. \end{aligned} \quad (13)$$

which expresses $[\partial_{(L)}G(0, x')]$ in terms of $G(0, x')$ as

$$\begin{aligned} \left(1 + \beta [\partial_{(L)}G_0(0, 0)]\right) [\partial_{(L)}G(0, x')] &= [\partial_{(L)}G_0(0, x')] - \alpha [\partial_{(L)}G_0(0, 0)] G(0, x') \\ &\quad - \beta [\partial_{(L,R)}^2 G_0(0, 0)] G(0, x'), \end{aligned} \quad (14)$$

or

$$\begin{aligned} [\partial_{(L)}G(0, x')] &= \left(1 + \beta [\partial_{(L)}G_0(0, 0)]\right)^{-1} \\ &\times \left([\partial_{(L)}G_0(0, x')] - \alpha [\partial_{(L)}G_0(0, 0)] G(0, x') - \beta [\partial_{(L,R)}^2 G_0(0, 0)] G(0, x')\right). \end{aligned} \quad (15)$$

Employing this result in Eq.(11), we have

$$\begin{aligned} G(0, x') &= G_0(0, x') - \alpha G_0(0, 0)G(0, x') - \beta [\partial_{(R)}G_0(0, 0)] G(0, x') \\ &\quad - \beta G_0(0, 0) \left(1 + \beta [\partial_{(L)}G_0(0, 0)]\right)^{-1} \left\{ [\partial_{(L)}G_0(0, x')] - \alpha [\partial_{(L)}G_0(0, 0)] G(0, x') \right. \\ &\quad \left. - \beta [\partial_{(L,R)}^2 G_0(0, 0)] G(0, x') \right\}, \end{aligned} \quad (16)$$

which yields $G(0, x')$ as

$$\begin{aligned} G(0, x') &= \left\{1 + \alpha G_0(0, 0) + \beta [\partial_{(R)}G_0(0, 0)] - \beta G_0(0, 0) \left(1 + \beta [\partial_{(L)}G_0(0, 0)]\right)^{-1} \right. \\ &\quad \left. \times \left(\alpha [\partial_{(L)}G_0(0, 0)] + \beta [\partial_{(L,R)}^2 G_0(0, 0)]\right)\right\}^{-1} \\ &\quad \times \left[G_0(0, x') - \beta G_0(0, 0) \left(1 + \beta [\partial_{(L)}G_0(0, 0)]\right)^{-1} [\partial_{(L)}G_0(0, x')]\right]. \end{aligned} \quad (17)$$

Eq. (17) may now be substituted into the right side of Eq. (15) to obtain $[\partial_{(L)}G(0, x')]$ in terms of G_0 and its derivatives alone. Finally, the substitution of these results for $G(0, x')$ and $[\partial_{(L)}G(0, x')]$ as indicated above into the right side of Eq. (11) yields the full, *exact* Green's function for the highly singular 1-D potential $U(x)$ of Eq. (2) joined onto any relatively well behaved 1-D potential $V(x)$, such as a harmonic oscillator and/or electric field potential independent of time. For the special case of $\beta = 0$, we obtain

$$G(x, x') = G_0(x, x') - \frac{\alpha G_0(x, 0)G_0(0, x')}{1 + \alpha G_0(0, 0)}. \quad (18)$$

3 The Role of Highly Singular Potentials in the 1-D Green's Function with a well-behaved potential $V(x)$

To examine the role of the highly singular potentials in the 1-D Green's function, we rewrite Eq. (4) in the form

$$G_0(x, x') = C(x')\{\eta_+(x' - x)y_1(x)y_2(x') + \eta_+(x - x')y_2(x)y_1(x')\} \quad (19)$$

where $\eta_+(x)$ is the Heaviside unit step function and $C(x') \equiv m(x')/\Delta(y_1, y_2)$. Since $\eta_+(0) = 1/2$,

$$G_0(0, 0) = C(0) \left\{ \frac{1}{2} y_1(0) y_2(0) + \frac{1}{2} y_2(0) y_1(0) \right\} = C(0) y_1(0) y_2(0). \quad (20)$$

Differentiating Eq. (19) to form $[\partial_{(L)} G_0(x, x')]$, there is a cancellation of terms involving Dirac delta functions arising from $\partial_{(L)} \eta_+(x - x')$, etc., and we obtain

$$[\partial_{(L)} G_0(x, x')] = C(x') \{ \eta_+(x' - x) y_1'(x) y_2(x') + \eta_+(x - x') y_2'(x) y_1(x') \}. \quad (21)$$

Differentiating again to form $[\partial_{(L,R)}^2 G(x, x')]$, we have

$$\begin{aligned} [\partial_{(L,R)}^2 G_0(x, x')] &= C'(x') \{ \eta_+(x' - x) y_1'(x) y_2(x') + \eta_+(x - x') y_2'(x) y_1(x') \} \\ &+ C(x') \left\{ \begin{aligned} &\delta(x' - x) y_1'(x) y_2(x') + \eta_+(x' - x) y_1'(x) y_2'(x') \\ &- \delta(x - x') y_2'(x) y_1(x') + \eta_+(x - x') y_2'(x) y_1'(x') \end{aligned} \right\}, \end{aligned} \quad (22)$$

which may be written more compactly using the definition of the Wronskian, $\Delta_{x'}(y_1, y_2)$, as (subscript "x'" denotes evaluation at x')

$$\begin{aligned} [\partial_{(L,R)}^2 G_0(x, x')] &= -C(x') \delta(x' - x) \Delta_{x'}(y_1, y_2) \\ &+ C(x') [\eta_+(x' - x) y_1'(x) y_2'(x') + \eta_+(x - x') y_2'(x) y_1'(x')] \\ &+ C'(x') \{ \eta_+(x' - x) y_1'(x) y_2(x') + \eta_+(x - x') y_2'(x) y_1(x') \}. \end{aligned} \quad (23)$$

Clearly, the first term on the right of Eq. (23) shows that

$$|[\partial_{(L,R)}^2 G_0(0, 0)]| \rightarrow \infty. \quad (24)$$

In view of the huge value of $|[\partial_{(L,R)}^2 G_0(0, 0)]|$, we may write Eq. (17) as

$$G(0, x') = -\frac{1 + \beta[\partial_{(L)} G_0(0, 0)]}{\beta^2 G_0(0, 0) [\partial_{(L,R)}^2 G_0(0, 0)]} \left\{ G_0(0, x') - \frac{\beta G_0(0, 0) [\partial_{(L)} G_0(0, x')]}{1 + \beta[\partial_{(L)} G_0(0, 0)]} \right\}, \quad (25)$$

and as long as we consider particle transmission through the highly singular potential at the origin (with $x < 0$ and $x' > 0$), this means that (Eq. (24))

$$G(0, x') = 0. \quad (26)$$

On the same basis Eq. (15) for $[\partial_{(L)} G(0, x')]$ may be written as

$$[\partial_{(L)} G(0, x')] = D^{-1} [\partial_{(L)} G_0(0, x')] + \frac{1}{\beta G_0(0, 0)} \left\{ G_0(0, x') - \beta D^{-1} G_0(0, 0) [\partial_{(L)} G_0(0, x')] \right\}, \quad (27)$$

where we have defined D as

$$D = 1 + \beta [\partial_{(L)} G_0(0, 0)]. \quad (28)$$

It should be noted that the role of the singular potential part $\Delta U = -\alpha \delta(x)$ is in fact, negligibly small when $\beta \neq 0$, as indicated in our earlier work proving that there is no particle transmission across the $\beta \delta'(x)$ - potential in the case of spatial translational invariance²². Here, we see that $\Delta U = -\alpha \delta(x)$ remains negligible in $G(x, x')$ for well behaved potentials $V(x)$ so long as $\beta \neq 0$:

$$\begin{aligned} G(x, x') &= G_0(x, x') - \beta G_0(x, 0) \left(D^{-1} [\partial_{(L)} G_0(0, x')] \right. \\ &\quad \left. + \frac{1}{\beta G_0(0, 0)} \left\{ G_0(0, x') - \beta D^{-1} G_0(0, 0) [\partial_{(L)} G_0(0, x')] \right\} \right), \end{aligned}$$

or

$$G(x, x') = G_0(x, x') - \frac{G_0(x, 0)G_0(0, x')}{G_0(0, 0)} \quad (29)$$

Considering that the Fourier transform of $G(x, x'; \omega)$ to direct time representation represents the quantum mechanical amplitude for a Schrödinger particle (wave packet) to be transmitted from position x' at time t' to x at a later time t , such that

$$\Psi_{out}(x, t) = \int \frac{d\omega}{\pi} e^{-i\omega(t-t')} \int_{-\infty}^{\infty} dx' G(x, x'; \omega) \Psi_{in}(x', t'), \quad (30)$$

it is clear that an electron wave packet, $\Psi_{in}(x' < 0, t')$ in the region of incidence, $x' < 0$, cannot be transmitted to $\Psi_{out}(x > 0, t)$ in the outgoing wave region, $x > 0$, on the other side of the highly singular potential $\beta\delta'(x)$ because Eq. (4) yields

$$\begin{aligned} G(x > 0, x' < 0; \omega) &= C(x') \left[y_1(x)y_2(x') - \frac{y_1(x)y_2(0)y_1(0)y_2(x')}{y_1(0)y_2(0)} \right] \\ &\equiv 0. \end{aligned} \quad (31)$$

This very general result means that there is *no* possibility of particle transmission from $x' < 0$ through the $\beta\delta'(x)$ - potential, even in the presence of well behaved potentials $V(x)$ as well as the presence of $\Delta U = -\alpha\delta(x)$.

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